

ON THE GROUND-STATE WAVE FUNCTION OF THE ONE-DIMENSIONAL POLARON IN THE STRONG-COUPLING LIMIT

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ABSTRACT. We consider the one-dimensional Fröhlich polaron localized in a symmetric decreasing electric potential. It is known that the non-linear Pekar functional corresponding to our model admits a unique minimizer. In the strong-coupling limit, we show that any approximate ground-state wave function of our model- after integrating out its phonon modes- converges in the weak sense to this unique minimizer.

1. INTRODUCTION

As a model of an electron moving in an ionic crystal, the polaron continues to be of interest. Because it is also one of the simplest examples of a particle interacting with a quantum field, it has served as a testing ground for various techniques in field theory (see [AlDe]) such as the Feynman path integral (see [Fy]). But despite the attention it has received over the last eight decades, many questions remain open. With a few exceptions in a limiting case (see e.g. [DoVa], [LiTh]), the polaron has eluded the exact calculation of the most basic quantities such as the effective mass and the ground state energy. Moreover, an exact analytic expression for the ground-state wave function of the model has yet to be given. In this paper, we give the first convergence result for the wave function.

Polaron theory began in the 1930s when ionic crystals of nonmetallic type- capable of producing strong electric fields- were being introduced into electronic devices (see [Pek]). Starting with L.D. Landau's paper [Ld] from 1933, where it was suggested that the electron deforms the crystal and traps itself in a hole of its own making, various models (see [Dev]) were developed to explain the transport of electrons through these crystals. These models were considerably more reliable for experiments than the standard band theory (see [Pek]), because they account for the polarization of the crystal due to the moving electron. This polarization is modelled in terms of the vibrational displacement of the ions in the crystal lattice; in the literature these vibrations are called *phonon modes*.

In 1937 H. Fröhlich suggested a model- known today as the *Fröhlich polaron*- to explain electrical breakdown in these crystals [Fr]. The Hamiltonian is

$$H_\alpha = \mathbf{p}^2 + \sum_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{\mathbf{k}} - \left(\frac{4\pi\alpha}{\Gamma} \right)^{\frac{1}{2}} \sum_{\mathbf{k}} \left[\frac{a_{\mathbf{k}}}{|\mathbf{k}|} e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{a_{\mathbf{k}}^\dagger}{|\mathbf{k}|} e^{-i\mathbf{k}\cdot\mathbf{x}} \right], \quad (1.1)$$

where $\mathbf{p} = -i\nabla$ (the electron momentum) and acts on $\mathcal{F} \otimes L^2(\mathbb{R}^3)$, where \mathcal{F} denotes the (symmetric) phonon Fock space. In (1.1) we use “ x ” to denote the electronic coordinate, “ k ” for the phonon mode and Γ for the volume of the crystal. The creation and annihilation operators $a_{\mathbf{k}}^\dagger$ and $a_{\mathbf{k}}$ are defined on \mathcal{F} with the canonical commutator relation $[a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger] = \delta(\mathbf{k} - \mathbf{k}')$. The coupling parameter $\alpha > 0$ was introduced by Fröhlich [Fr-2] in 1954 to describe the interaction between the electron and the phonon modes. The model is also known as the *large polaron*, because the spatial extension of the wave function is larger than the crystal lattice spacing. Therefore a continuum approximation $\sum_{\mathbf{k}} \rightarrow \Gamma(2\pi)^{-3} \int d^3k$ for the Hamiltonian in (1.1) is also allowed.

A proof of the self-adjointness for Hamiltonians of this type was first given in 1964 by E. Nelson [Ne].

The *ground state energy* of the model is

$$E_\alpha = \inf \{ \langle \Psi, H_\alpha \Psi \rangle_{\mathcal{F} \otimes L^2(\mathbb{R}^3)} \mid \Psi \in \mathcal{F} \otimes L^2(\mathbb{R}^3) \text{ and } \|\Psi\|_{\mathcal{F} \otimes L^2(\mathbb{R}^3)} = 1 \}, \quad (1.2)$$

where the operator H_α is the Hamiltonian in (1.1). A normalized wave function in $\mathcal{F} \otimes L^2(\mathbb{R}^3)$ that achieves the ground state energy in (1.2) is a *ground-state wave function*.

The mathematical difficulty in calculating the ground state energy and the ground-state wave function of the model stems from the electron-phonon interaction term of the Hamiltonian in (1.1). Not only are the electron and phonon co-ordinates in (1.1) inseparable, but we also do not *a priori* know the explicit dependence between the co-ordinates. The minimization problem in (1.2) is therefore intractable.

During the 1950s this mathematical difficulty motivated physicists to develop various techniques for approximating the ground state energy in (1.2) by exploiting the properties of the ground-state wave function. In his 1951 monograph [Pek] S.I. Pekar presents a non-linear theory posited on his *Produkt-Ansatz* for the ground-state wave function. Based on his physical intuition that the phonons are not sensitive to the instantaneous position of the electron, Pekar proposed that the ground-state wave function in (1.2) can be expressed in the product form

$$\Psi = |\phi\rangle \otimes |\zeta\rangle. \quad (1.3)$$

In (1.3) $|\zeta\rangle \in \mathcal{F}$ is a coherent state defined only on the phonon co-ordinates, and $\phi \in L^2(\mathbb{R}^3)$ is a normalized, electronic wave function. In particular, $\alpha^{-\frac{3}{2}}\phi(\frac{x}{\alpha})$ is a minimizer of the non-linear problem:

$$e_P = \inf \left\{ \int_{\mathbb{R}^3} |\nabla \phi|^2 d\mathbf{x} - \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{\phi(\mathbf{x})^2 \phi(\mathbf{y})^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y} \mid \int_{\mathbb{R}^3} \phi(\mathbf{x})^2 d\mathbf{x} = 1 \right\}. \quad (1.4)$$

Pekar's ansatz in (1.3) offers the computational advantage of eliminating all of the phonon co-ordinates in the optimization problem from (1.2) for the ground state energy. Minimizing $\langle \Psi, H_\alpha \Psi \rangle$ over the more restrictive set of product wave functions in (1.3) yields the following *upper bound* for the true ground state energy:

$$E_\alpha \leq \inf \{ \langle \Psi, H_\alpha(V) \Psi \rangle_{\mathcal{F} \otimes L^2(\mathbb{R}^3)} \mid \|\Psi\|_{\mathcal{F} \otimes L^2(\mathbb{R}^3)} = 1 \text{ and } \Psi = |\phi\rangle \otimes |\zeta\rangle \} \quad (1.5)$$

$$= \alpha^2 e_P, \quad (1.6)$$

with the *Pekar energy* e_P as defined in (1.4). Numerical work in 1976 by S.J. Miyake suggests that $e_P = -0.108513$ [My].

Pekar's ansatz gives rise to a widely studied minimization problem with a non-linear energy functional, given in (1.4) above, known as the *Pekar functional* (see eg. [GrHtWl], [Li], [Ln], [Ln-2] and [LwRg]). That a minimizer actually exists for the non-linear problem in (1.4) has been shown only in 1977 by E.H. Lieb using rearrangement inequalities [Li]. Lieb has also established that this minimizer is unique up to translations by proving that there is a unique solution for the corresponding Euler-Lagrange equation:

$$\left\{ -\Delta - 2 \int_{\mathbb{R}^3} |\phi(y)|^2 |x - y|^{-1} dy \right\} \phi(x) = \lambda \phi(x). \quad (1.7)$$

The equation in (1.7) is known as the *Choquard-Pekar* or the *Schrödinger-Newton* equation, and it has attracted a lot of attention in the recent literature (see eg. [GmVs], [LwRg], [Lz], [MzVs], [MzVs-2], [MzVs-3], [MzVs-4], [MzVs-5] and [Rd]). In particular, E. Lenzmann has shown that around the unique minimizer $Q(x)$ of the Choquard-Pekar equation in (1.7), the linearization

$$L_+ \zeta = -\Delta \zeta + \lambda \zeta - (|x|^{-1} * |Q|^2) \zeta - 2Q (|x|^{-1} * (Q\zeta))$$

has a non-degenerate kernel [Lz]:

$$\ker L_+ = \text{span}\{\partial_{x_1} Q, \partial_{x_2} Q, \partial_{x_3} Q\}. \quad (1.8)$$

With this non-degeneracy result, Lenzmann establishes the uniqueness up to translations of the *pseudo-relativistic version* of the Choquard-Pekar equation via an implicit function-type argument [Lz]. Lenzmann's non-degeneracy result in (1.8) has found many applications (see [Rd] and the references therein), and it is a crucial ingredient, for example, in the proof of the symmetry of the bipolaron bound state given by Frank, Lieb and Seiringer in [FrLiSr]. These uniqueness and non-degeneracy results have been extended to the anisotropic polaron (see [LwRg]) by J. Ricaud in recent work [Rd].

Despite the mathematical interest that the Pekar functional continues to stimulate, it was noticed already in the 1950s that Pekar's ansatz is only physically sensible for describing crystals with a very large ("strong") coupling parameter α [Fr-2]. And a more adequate theory was needed to explain the transport of electrons in weak-coupling crystals (eg. InSb; cf. [Dev]). In 1954 Fröhlich has introduced a weak-coupling theory (see [Fr-2]) based on the canonical transformation of T.D. Lee, F.E. Low and D. Pines from 1953 [LLP]. This in turn motivated R.P. Feynman in 1955 to use the path integral to develop an intermediate-coupling theory that is applicable to a wider range of coupling parameters [Fy].

These theories- each useful at different values of the coupling parameter- only provide an upper bound for the true ground state energy E_α in (1.2). In 1958, however, E.H. Lieb and K. Yamazaki arrive at a rigorous lower bound for the ground state energy via modifying the Hamiltonian (1.1) rather than making an ansatz about the ground-state wave function [LiYa]. Their lower bound, however, differs from Pekar's upper bound in (1.6) by a factor of 3, so their calculation unfortunately does not yield the exact ground state energy in the strong-coupling limit. Lieb and Yamazaki's techniques from 1958 nevertheless continue to inspire rigorous calculations in strong-coupling theory: commutator estimates with their vector operator $\mathbf{Z} = (Z_1, Z_2, Z_3)$, where

$$Z_j = \left(\frac{4\pi\alpha}{\Gamma} \right)^{\frac{1}{2}} \sum_{|\mathbf{k}| > K} k_j \frac{a_{\mathbf{k}}}{|\mathbf{k}|^3} e^{i\mathbf{k} \cdot \mathbf{x}}, \quad j = 1, 2, 3,$$

are necessary when using an ultraviolet cutoff on Hamiltonians such as that in (1.1) (see eg. [AnLa], [BeBl], [FrGs], [FrSl] and [LiTh]). It is also useful in quantum electrodynamics (see proof of Corollary 2.2 in [LiLo-2]).

To this day it is not known how to calculate the exact ground state energy at finite values of the coupling parameter α , but in 1981 M.D. Donsker and S.R.S. Varadhan have succeeded in using techniques from large deviation theory to show that Pekar's approximation ((1.5), (1.6)) of the ground state energy is exact in the strong-coupling limit [DoVa]:

$$\lim_{\alpha \rightarrow \infty} \frac{E_\alpha}{\alpha^2} = e_P. \quad (1.9)$$

Of course, e_P is the upper bound from (1.4) that is calculated using Pekar's ansatz for the ground-state wave function. In 1995 E.H. Lieb and L.E. Thomas provide an alternate, pedestrian proof of (1.9) using simple modifications of the Hamiltonian, a philosophy that can be traced back to the earlier work [LiYa] of Lieb and Yamazaki from 1958. In [LiTh] Lieb and Thomas use coherent states to obtain an agreeable lower bound, and the strategy also yields a rate of convergence for the result in (1.9). Their technique has motivated recent study of the ground state energy of multi-polaron systems (see [AnLa], [BeBl] and [GrMl]) and can also be adapted to other models (see [FrGs] for the polaron in a large magnetic field). We use their methods to argue the exact ground state energy of our one-dimensional model (see Theorem 1 below).

1.1. Motivation. Showing Pekar's product wave function yields the exact ground state energy in the strong-coupling limit is a successful chapter in polaron theory, spanning more than four decades. This by no means is a justification of Pekar's ansatz for the ground-state wave function, which, as Lieb and Yamazaki point out in 1958, is in fact inadequate for calculating the expectation values of various operators at the ground state. For example, the expectation value $\langle H_\alpha^2 \rangle = \infty$ when one takes the ground-state wave function to be Pekar's product function in (1.3). It still remains to understand the connection between the true ground-state wave function and Pekar's product wave function.

With this paper we present a strategy that can be used to show that in the limit $\alpha \rightarrow \infty$ the true ground-state wave function of the Fröhlich Hamiltonian- after integrating out its phonon modes- converges (in the weak sense) to the electronic wave function in Pekar's ansatz. As evident from (1.4), this electronic wave function is the minimizer of the corresponding non-linear Pekar functional.

A much stronger relationship between the ground state of the Fröhlich Hamiltonian and the product wave function from Pekar's ansatz in (1.3) has been recently conjectured by E.H. Lieb and R. Seiringer [LiSr].

To have a well-defined notion of convergence, however, we need to ensure that the corresponding Pekar functional admits a unique minimizer. Note that the Pekar energy functional in (1.4), originally studied by Lieb in [Li], has translational invariance. To even have a chance at uniqueness we must break translation invariance by introducing a localizing electric potential (in the \mathbf{x} co-ordinate only) for the system: for some $V(\mathbf{x}) \geq 0$ that vanishes at infinity, consider the localized Hamiltonian

$$H_\alpha(V) \equiv H_\alpha - \alpha^2 V(\alpha \mathbf{x}), \quad (1.10)$$

where H_α is the translation invariant Hamiltonian from (1.1). The corresponding Pekar energy functional is

$$\mathcal{E}_V(\phi) = \int_{\mathbb{R}^3} \left(|\nabla \phi|^2 - V(\mathbf{x}) |\phi(\mathbf{x})|^2 \right) d\mathbf{x} - \int \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x} - \mathbf{y}|} d\mathbf{x} d\mathbf{y}. \quad (1.11)$$

In 1977 E.H. Lieb proved uniqueness *up to translations* [Li] for the functional in (1.4) (see also "Appendix A" in [Lz] for a somewhat different proof), but his proof exploits some essential scaling relations that are no longer true for the functional in (1.11), where we break translational invariance of the system with a

localizing potential. The existence of a minimizer for the Pekar functional with the inclusion of an external potential, (1.11), has been studied by P.L. Lions in the 1980s when developing his compactness arguments (see [Ln] and [Ln-2] and cf. [Li-2], an earlier similar result of E.H. Lieb). In the presence of a localizing potential, while existence issues can now be settled using Lions' concentration compactness lemma [Ln], we are not aware of any tools for addressing the uniqueness of the minimizer. Even when the localizing potential in (1.11) is the Coulomb potential, $|x|^{-1}$, we are unable to adapt the technique from [Li].

A uniqueness result is available only in one-dimension (see [JjSt] and [MlStTr]), so we can only provide rigorous arguments for a one-dimensional model. But we emphasize that there is nothing intrinsically one-dimensional about our strategy, which follows from a very simple application of the variational principle.

2. THE ONE-DIMENSIONAL MODEL AND STATEMENT OF RESULTS

We work with the one-dimensional Fröhlich polaron localized in a *symmetric decreasing*, $C^1(\mathbb{R})$ electric potential $V(x) \geq 0$ that *vanishes at infinity*. The Hamiltonian for our model,

$$H_\alpha(V) = -\frac{d^2}{dx^2} + \sum_{|k|>0} a_k^\dagger a_k - \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k|>0} \left[a_k e^{ikx} + a_k^\dagger e^{-ikx} \right] - \alpha^2 V(\alpha x), \quad (2.1)$$

is defined on $\mathcal{F} \otimes L^2(\mathbb{R})$, where \mathcal{F} is a symmetric Fock space over $\ell^2(\mathbb{Z}/L)$. In (2.1) we use “ x ” to denote the electronic coordinate, “ k ” for the phonon mode, “ $2L$ ” is the length of the crystal and “ $\frac{1}{L}$ ” is the lattice spacing. The creation and annihilation operators a_k^\dagger and a_k are defined on \mathcal{F} with the canonical commutator relation $[a_k, a_{k'}^\dagger] = \delta(k - k')$. As usual the continuum approximation “ $\sum_k \rightarrow L \int dk$ ” is allowed.

The ground state energy of the model is defined as

$$E_\alpha(V) = \inf \{ \langle \Psi, H_\alpha(V) \Psi \rangle_{\mathcal{F} \otimes L^2} \mid \|\Psi\|_{\mathcal{F} \otimes L^2} = 1 \}, \quad (2.2)$$

and an optimizing function in (2.2) is the ground state wave function of the model. As with the three-dimensional case discussed above, it is straightforward to calculate with Pekar's *Produkt-Ansatz* (see (1.3) above) for the ground-state wave function

$$\Psi = |u\rangle_{L^2(\mathbb{R})} \otimes |\zeta\rangle_{\mathcal{F}}, \quad (2.3)$$

that

$$E_\alpha(V) \leq \alpha^2 e(V). \quad (2.4)$$

A scaled version of the electronic wave function in Pekar's ansatz, $\alpha^{-\frac{1}{2}} u(\frac{x}{\alpha})$, is a minimizer of the one-dimensional minimization problem for the Pekar energy $e(V)$:

$$e(V) = \inf \{ \mathcal{E}_V(u) : \int_{\mathbb{R}} u^2 dx = 1 \}, \quad (2.5)$$

with the one-dimensional Pekar functional:

$$\mathcal{E}_V(u) = \int_{\mathbb{R}} (u'^2 - u^4 - V(x)u^2) dx. \quad (2.6)$$

When $V = 0$, it has been shown that $e(0) = -\frac{1}{12}$ (see e.g. [Gh]). Since V is a localizing potential, $e(V) < 0$.

The one-dimensional polaron was introduced by E.P. Gross in his 1976 paper as a toy model [Go]. But it has since attracted sizeable attention in the literature and is not entirely artificial (see eg. [FrGs], [FrLiSrTh], [Gn], [KoLeSm], [Mn], [PtSm], [SKVPD], [Sp], [Sp-2], [VPSD]). The most compelling reason to study the one-dimensional model is its connection to the three-dimensional polaron in a magnetic field, also known as the *magneto-polaron*. In 1992 E.A. Kochetov, H. Leschke and M.A. Smondyrev [KoLeSm] consider a three-dimensional polaron in a strong magnetic field \mathbf{B} and with some fixed coupling $\alpha > 0$. In the limit $|\mathbf{B}| \rightarrow \infty$, they argue that the dynamics of the three-dimensional magneto-polaron is equivalent to that of a one-dimensional strong-coupling polaron with the large coupling constant $\alpha' = (\alpha \ln |\mathbf{B}|)/2$.

But Kochetov et. al's argument- reminiscent of Pekar's heuristic justification [Pek] of his *Produkt-Ansatz*- has been rigorously verified only recently by R.L. Frank and L. Geisinger in [FrGs]. They calculate the exact ground state energy of the magneto-polaron and use the one-dimensional version of the strategy developed in [LiTh]. We present this one-dimensional version in full detail in order to calculate the exact ground state energy of our model. We also think this calculation conveniently complements Frank and Geisinger's argument in Section 6 of their paper [FrGs].

Theorem 1. *For the ground state energy $E_\alpha(V)$ in (2.2) and the Pekar energy $e(V)$ in (2.5),*

$$\lim_{\alpha \rightarrow \infty} \frac{E_\alpha(V)}{\alpha^2} = e(V).$$

The first natural task is to see that a true ground-state wave function exists. While there are existence results in the literature (see [Sp] [Sp-2], [Sp-3], [GrLo] and [GrLo-2]), we circumvent this important issue by using our result in Theorem 1 to define the notion of an *approximate ground-state wave function*.

Definition 2. A wave function $\Psi_\alpha \in \mathcal{F} \otimes L^2(\mathbb{R})$ is an *approximate ground-state wave function* for the localized Hamiltonian $H_\alpha(V)$ in (2.1) if $\|\Psi_\alpha\|_{\mathcal{F} \otimes L^2(\mathbb{R})} = 1$ and

$$\langle \Psi_\alpha, H_\alpha(V) \Psi_\alpha \rangle_{\mathcal{F} \otimes L^2(\mathbb{R})} - E_\alpha(V) = o(\alpha^2). \quad (2.7)$$

If a true ground-state wave function exists, it is obviously also an approximate ground-state wave function. From Theorem 1 we see that Pekar's product wave function in (2.3) is also an approximate ground-state wave function. We will show that *any* approximate ground-state wave function of our model converges in the weak sense to the *unique* minimizer of the corresponding Pekar functional given in (2.6).

Because the potential $V(x)$ is symmetric decreasing and vanishes at infinity, it can easily be shown using the direct method in the calculus of variations that a minimizer exists for the minimization problem in (2.5) (see Theorem 8.6 and Chapter 11 in [LiLo]; see also [Gh]). The argument is very similar to our proof of Lemma 5 below. A minimizer is also real-valued and positive (cf. Theorem 7.8 in [LiLo]).

To argue uniqueness we consider the Euler-Lagrange equation. Any minimizer of the problem in (2.5) is a positive, real-valued solution of the eigenvalue equation

$$-u'' - 2u^3 - Vu = \lambda u, \quad (2.8)$$

where $\lambda \in \mathbb{R}$ is a Lagrange multiplier corresponding to the constraint $\int_{\mathbb{R}} u^2 dx = 1$ in (2.5). It can be argued with the standard tools in regularity theory (Theorem 11.7 in [LiLo]; see also [Gh]) that the solution of (2.8) is in fact a classical solution. If there are two minimizers for the problem in (2.5), then they each satisfy (2.8) with possibly different values of λ . To show that our one-dimensional Pekar functional from (2.5) admits a unique minimizer, we must see that over all non-negative $u \in L^2(\mathbb{R})$ with $\int_{\mathbb{R}} u^2 dx = 1$ there is only one pair (λ, u) which satisfies the equation in (2.8). We see this from Theorem 3 in [JjSt] and Theorem 2.1 in [MlStTr]:

Proposition 3. *If $V \in C^1(\mathbb{R})$ is a nonzero, nonnegative and symmetric decreasing function that vanishes at infinity, then the one-dimensional minimization problem in (2.5) for the Pekar energy $e(V)$ admits a unique minimizer.*

We briefly describe their proofs. First, consider the lowest eigenvalue of the linearization of the equation in (2.8):

$$\lambda_0 = \inf \left\{ \int_{-\infty}^{+\infty} (u')^2 - V(x)u^2 dx : u \in H^2(\mathbb{R}) \text{ and } \int_{-\infty}^{\infty} u^2 dx = 1 \right\}. \quad (2.9)$$

In 1999, H. Jeanjean and C.A. Stuart bifurcate (see Theorem 3 in [JjSt]) a unique continuous curve of solutions $u \in C^1((-\infty, \lambda_0), \lambda)$ such that for each $\lambda \in (-\infty, \lambda_0)$, the pair $(\lambda, u(\lambda))$ is a solution of (2.8). They argue that all solutions of (2.8) belong to this curve:

$$\{(\lambda, u(\lambda)) : \lambda \in (-\infty, \lambda_0)\} = \{(\mu, \nu) : (\mu, \nu) \text{ is a solution to (2.8)}\}.$$

This means that for each $-\infty < \lambda < \lambda_0$, there is a unique $u(\lambda)$ that satisfies (2.8). In 2003 J.B. McLeod, C.A. Stuart and W.C. Troy show (Theorem 2.1 in [MlStTr]) that $\|u(\lambda)\|_{L^2(\mathbb{R})}$ decreases as λ increases from $-\infty$ to λ_0 . Therefore, there is only one pair $(\lambda, u(\lambda))$ that satisfies (2.8) with $\|u(\lambda)\|_2 = 1$, and this is the unique minimizer of our problem in (2.5).

After bifurcating a curve of solutions from the lowest eigenvalue λ_0 in (2.9), the strategy in [JjSt] is to repeatedly use the implicit function theorem at the positive solutions to get a global branch containing all the positive, real-valued solutions of the equation in (2.8). As it was pointed out to the author by Professor C.A. Stuart, the uniqueness result is limited to one-dimension, because the authors in [JjSt] can only see how to check the hypotheses of the implicit function theorem in the one-dimensional case. Local bifurcation

at the lowest eigenvalue is possible in all dimensions since the eigenvalue is always simple (cf. [CrRa]), but global continuation is the main problem.

With this uniqueness result we have a well-defined notion of convergence, and we now state our main result.

(In this paper, we say a Borel measure W is *bounded* if $\int_{\mathbb{R}} W(x)dx = 1$. An example is the Dirac-delta measure.)

Theorem 4. *Let u_V be the unique minimizer of the minimization problem in (2.5), and let $\Psi_\alpha \in \mathcal{F} \otimes L^2(\mathbb{R})$ be any approximate ground-state wave function of the Hamiltonian in (2.1). Then:*

$$\lim_{\alpha \rightarrow \infty} \int_{\mathbb{R}} \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\cdot}{\alpha} \right)\|_{\mathcal{F}}^2 \right] W(x)dx = \int_{\mathbb{R}} |u_V|^2 W(x)dx \quad (2.10)$$

for any bounded Borel measure $W(x)$ on the real line.

2.1. Strategy. Let δ be a real parameter and $W(x)$ some bounded Borel measure as above. The main idea, suggested to the author by Professor R.L. Frank, is to perturb the Hamiltonian $H_\alpha(V)$ in (2.1):

$$H_\alpha(V + \delta W) \equiv H_\alpha(V) + \alpha^2 \delta W(\alpha x). \quad (2.11)$$

Imitating the proof of Theorem 1, we calculate the exact ground state energy of the “perturbed Hamiltonian” in (2.11):

$$E_\alpha(V + \delta W) = \alpha^2 e(V + \delta W), \quad (2.12)$$

$$e(V + \delta W) \equiv \inf \left\{ \mathcal{E}_{V+\delta W}(u) : \int_{\mathbb{R}} u^2 dx = 1 \right\}, \quad (2.13)$$

where

$$\mathcal{E}_{V+\delta W}(u) \equiv \mathcal{E}_V(u) + \delta \int_{\mathbb{R}} W(x)|u|^2 dx. \quad (2.14)$$

Of course the Pekar functional \mathcal{E}_V was already defined in (2.5), and from Proposition 3 we know it admits a unique minimizer u_V .

Let Ψ_α be an approximate ground-state wave function of the Hamiltonian $H_\alpha(V)$. Since Ψ_α is not necessarily the ground-state wave function of the perturbed Hamiltonian $H_\alpha(V + \delta W)$, a simple application of the variational principle yields

$$\begin{aligned} E_\alpha(V + \delta W) &\leq \langle \Psi_\alpha, [H_\alpha(V + \delta W)] \Psi_\alpha \rangle \\ &= \langle \Psi_\alpha, H_\alpha(V) \Psi_\alpha \rangle + \alpha^2 \delta \langle \Psi_\alpha, W(\alpha x) \Psi_\alpha \rangle \\ &\leq E_\alpha(V) + o(\alpha^2) + \alpha^2 \delta \langle \Psi_\alpha, W(\alpha x) \Psi_\alpha \rangle, \end{aligned}$$

where the inner product is on $\mathcal{F} \otimes L^2(\mathbb{R})$.

Dividing by α^2 and using Theorem 1, (2.12) and (2.13) we see that

$$\frac{e(V + \delta W) - e(V)}{\delta} = \lim_{\alpha \rightarrow \infty} \int_{\mathbb{R}} \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\cdot}{\alpha} \right)\|_{\mathcal{F}}^2 \right] W(x) dx. \quad (2.15)$$

Then our main result (2.10) in Theorem 4 above follows directly from (2.15) if we can differentiate the “perturbed Pekar energy” $e(V + \delta W)$ at $\delta = 0$:

Lemma 5. *Suppose the one-dimensional minimization problem in (2.5) for the Pekar energy $e(V)$ admits a unique minimizer u_V . Let $W(x)$ be any bounded Borel measure on the real line, and let $e(V + \delta W)$ be the perturbed Pekar energy defined in (2.13) with some real parameter δ . Then the map $\delta \mapsto e(V + \delta W)$ is differentiable at $\delta = 0$ and*

$$\left. \frac{d}{d\delta} \right|_{\delta=0} e(V + \delta W) = \int_{\mathbb{R}} W(x) |u_V|^2 dx.$$

The proof of Lemma 5- which we provide in Section 4 below- again follows from a simple application of the variational principle and a compactness argument (Theorem 8.6 in [LiLo]).

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3. EXACT GROUND STATE ENERGY: PROOF OF THEOREM 1

In this section we will calculate the exact ground state energy of our one-dimensional model using the strategy developed in [LiTh].

We use $\langle H \rangle$ to denote the expectation value of the operator on $\mathcal{F} \otimes L^2(\mathbb{R})$. Likewise, $\|\Psi\|$ should be read: $\|\Psi\|_{\mathcal{F} \otimes L^2(\mathbb{R})}$.

The main idea in this proof is to work with a rigorously justified approximation that the electron only interacts with finitely many phonon modes and to then use coherent states to arrive at a lower bound that agrees- to the leading order in α - with Pekar's upper bound in (2.4). This already departs from the physical picture offered by Pekar's ansatz, that the phonons cannot follow the electron.

The general utility of coherent states for obtaining rigorous (lower) bounds is discussed in [LiSrYg] and [Li-3].

3.1. Ultraviolet Cutoff. We ignore large modes in the Fröhlich Hamiltonian and work on a reduced mode space $\{k : |k| \leq K\}$ with a cutoff Hamiltonian

$$H_K = (1 - \epsilon)p^2 + \sum_{|k| \leq K} a_k^\dagger a_k - \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k| \leq K} \left(a_k e^{ikx} + a_k^\dagger e^{-ikx} \right) - \alpha^2 V(\alpha x) \quad (3.1)$$

The parameters ϵ and K will be chosen at the very end of the computations.

We bound the energy of the Fröhlich Hamiltonian from below with the energy of the *cutoff Hamiltonian* H_K in (3.1). We observe

$$H_\alpha(V) = H_K + \epsilon p^2 + \sum_{|k| > K} a_k^\dagger a_k - \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k| > K} \left(a_k e^{ikx} + a_k^\dagger e^{-ikx} \right) \quad (3.2)$$

and we will arrive at a lower bound by making an estimate on the interaction term in (3.2).

We use a standard commutator identity $\langle [p, a_k e^{ikx}] \rangle = k \langle a_k e^{ikx} \rangle$ and work with two operators $Z = \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k| > K} \frac{a_k e^{ikx}}{k}$ and $Z^\dagger = \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k| > K} \frac{a_k^\dagger e^{-ikx}}{k}$.

For any $0 < \epsilon < 1$,

$$\begin{aligned} \left\langle \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k| > K} \left(a_k e^{ikx} + a_k^\dagger e^{-ikx} \right) \right\rangle &= \langle [p, Z - Z^\dagger] \rangle \\ &\leq 2 \langle p^2 \rangle^{\frac{1}{2}} \langle -(Z - Z^\dagger)^2 \rangle^{\frac{1}{2}} \\ &\leq \epsilon \langle p^2 \rangle + \frac{1}{\epsilon} \langle -(Z - Z^\dagger)^2 \rangle \\ &\leq \epsilon \langle p^2 \rangle + \frac{2}{\epsilon} \langle ZZ^\dagger + Z^\dagger Z \rangle \end{aligned} \quad (3.3)$$

$$\begin{aligned} &= \epsilon \langle p^2 \rangle + \frac{2}{\epsilon} \langle [Z, Z^\dagger] \rangle + \frac{4}{\epsilon} \langle Z^\dagger Z \rangle \\ &\leq \epsilon \langle p^2 \rangle + \frac{4\alpha}{\epsilon K} + \frac{8\alpha}{\epsilon K} \left\langle \sum_{|k| > K} a_k^\dagger a_k \right\rangle \end{aligned} \quad (3.4)$$

Above, (3.3) is immediate from the positive definiteness of $(Z + Z^\dagger)^2$. To arrive at (3.4), we make the following estimates on $\langle Z^\dagger Z \rangle$ and $\langle [Z, Z^\dagger] \rangle$:

$$\begin{aligned} \langle Z^\dagger Z \rangle &= \left(\frac{\alpha}{L}\right) \sum_{|k| > K} \sum_{|k'| > K} \left\langle \frac{a_k^\dagger a_{k'} e^{i(k' - k)x}}{kk'} \right\rangle \\ &\leq \left(\frac{\alpha}{L}\right) \left(\sum_{|k| > K} \frac{1}{k} \langle a_k^\dagger a_k \rangle^{\frac{1}{2}} \right)^2 \end{aligned}$$

$$\begin{aligned}
&\leq \left(\frac{\alpha}{L}\right) \left(\sum_{|k|>K} \frac{1}{|k|^2}\right) \left(\sum_{|k|>K} \langle a_k^\dagger a_k \rangle\right) \\
&\leq \frac{2\alpha}{K} \left\langle \sum_{|k|>K} a_k^\dagger a_k \right\rangle
\end{aligned}$$

Since $[a_k, a_{k'}^\dagger] = \delta_{kk'}$,

$$\begin{aligned}
\langle [Z, Z^\dagger] \rangle &= \left(\frac{\alpha}{L}\right) \sum_{|k|>K} \sum_{|k'|>K} \left\langle \frac{e^{i(k-k')x} (a_k a_{k'}^\dagger - a_{k'}^\dagger a_k)}{kk'} \right\rangle \\
&\leq \left\langle \frac{2\alpha}{K} \right\rangle
\end{aligned}$$

We can now construct a lower bound from (3.2):

$$\langle H_\alpha(V) \rangle \geq \langle H_K \rangle + \left(1 - \frac{8\alpha}{\epsilon K}\right) \left\langle \sum_{|k|>K} a_k^\dagger a_k \right\rangle - \left\langle \frac{4\alpha}{\epsilon K} \right\rangle$$

Clearly, we require from our parameters ϵ and K that $1 = \frac{8\alpha}{\epsilon K}$. We now arrive at our lower bound:

$$E_\alpha(V) \geq \inf_{\|\Psi\|=1} \langle \Psi, H_K \Psi \rangle - \frac{1}{2}.$$

In sharp contrast to the three-dimensional computation performed in [LiTh], our error term, $-\frac{1}{2}$, does not depend on the cutoff parameter K .

3.2. Localizing the Electron. We will bound *from below* the ground state energy of the cutoff Hamiltonian H_K : $\inf_{\|\Psi\|=1} \langle \Psi, H_K \Psi \rangle$ (given in (3.1)).

Here, $(\Delta E) > 0$ is a parameter whose specific value will be given at the very end of the computations. We will denote by $\inf'_{\|\Psi\|} \langle \Psi, H_K \Psi \rangle$ the infimum taken over all wave functions whose *electronic coordinate is localized* in an interval of length $\frac{\pi}{(\Delta E)^{\frac{1}{2}}}$. This restriction, we argue, increases the ground state energy of H_K by at most ΔE :

$$\inf_{\|\Psi\|=1} \langle \Psi, H_K \Psi \rangle \geq \inf'_{\|\Psi\|=1} \langle \Psi, H_K \Psi \rangle - (\Delta E) \tag{3.5}$$

Let $\|\Psi\| = 1$ and $E = \langle \Psi, H_K \Psi \rangle$. We define $\phi(x) = \cos\left((\Delta E)^{\frac{1}{2}}x\right)$ on its support in $\left(-\frac{\pi}{2(\Delta E)^{\frac{1}{2}}}, \frac{\pi}{2(\Delta E)^{\frac{1}{2}}}\right)$ and write $\phi_y(x) = \phi(x - y)$. To argue (3.5), it suffices to show for some $\bar{y} \in \mathbb{R}$,

$$\frac{\langle (\phi_{\bar{y}} \Psi), H_K (\phi_{\bar{y}} \Psi) \rangle}{\langle \phi_{\bar{y}} \Psi, \phi_{\bar{y}} \Psi \rangle} \leq E + (\Delta E). \tag{3.6}$$

A direct calculation gives $\int_{\mathbb{R}} \langle (\phi_y \Psi), H_K (\phi_y \Psi) \rangle dy = \int (\phi')^2 + E\phi^2 dx$ and

$$\begin{aligned}
&\int_{\mathbb{R}} (\langle (\phi_y \Psi), H_K (\phi_y \Psi) \rangle - (E + \Delta E) \langle \phi_y \Psi, \phi_y \Psi \rangle) dy \\
&= \int_{-\frac{\pi}{2(\Delta E)^{\frac{1}{2}}}}^{\frac{\pi}{2(\Delta E)^{\frac{1}{2}}}} (\phi')^2 - (\Delta E)\phi^2 dx = 0
\end{aligned}$$

since (ΔE) is the Dirichlet energy of ϕ . So there exists some $\bar{y} \in \mathbb{R}$ such that (4.6) holds. From now on, we consider the electron to be localized in some interval of length $\frac{\pi}{(\Delta E)^{\frac{1}{2}}}$.

3.3. Block Hamiltonian. We now decompose our finite mode space into finitely many blocks: $\{k : |k| < K\} = \bigcup_n \{B_n\}$; each block B_n contains “ PL ” modes where “ $\max_{k_i, k_j \in B_n} |k_i - k_j| = P$ ” is the size of each block.

On each block B_n we analogously define block annihilation and creation operators: $A_{B_n} = \frac{1}{(PL)^{\frac{1}{2}}} \sum_{k \in B_n} a_k$ and $A_{B_n}^\dagger = \frac{1}{(PL)^{\frac{1}{2}}} \sum_{k \in B_n} a_k^\dagger$. Clearly, $[A_{B_m}, A_{B_n}^\dagger] = \delta_{mn}$. On each block B_n , we see from the Cauchy-Schwarz inequality that

$$A_{B_n}^\dagger A_{B_n} \leq \sum_{k \in B_n} a_k^\dagger a_k. \quad (3.7)$$

For reasons that will become clear in the next stage of the computation, we now want to work with the approximation that the electron interacts with at most one mode k_{B_n} in each block B_n . For this approximation to work, we make the following estimate on the interaction term of our cutoff Hamiltonian: for any parameter $0 < \delta < 1$ and any mode k_{B_n} in each block B_n , completing the square yields

$$\begin{aligned} & \left\langle \left(\frac{\alpha}{L} \right)^{\frac{1}{2}} \sum_{B_n} \sum_{k \in B_n} \left[a_k (e^{ik_{B_n}x} - e^{ikx}) + a_k^\dagger (e^{-ik_{B_n}x} - e^{-ikx}) \right] \right\rangle \\ & \leq \left\langle \delta \sum_{|k| < K} a_k^\dagger a_k + \left(\frac{\alpha}{L} \right) \frac{1}{\delta} \sum_{B_n} \sum_{k \in B_n} |e^{ik_{B_n}x} - e^{ikx}|^2 \right\rangle \\ & \leq \left\langle \delta \sum_{|k| < K} a_k^\dagger a_k + \left(\frac{\alpha}{L} \right) \frac{1}{\delta} \sum_{B_n} \sum_{k \in B_n} |k - k_{B_n}|^2 |x|^2 \right\rangle \\ & \leq \left\langle \delta \sum_{|k| < K} a_k^\dagger a_k \right\rangle + \frac{2\alpha K P^2 \pi^2}{\delta(\Delta E)}. \end{aligned} \quad (3.8)$$

To arrive at (3.8), we used the rigorously justified approximation (see (3.5)) that the electronic co-ordinate is localized in an interval of length $\frac{\pi}{(\Delta E)^{\frac{1}{2}}}$.

The parameters P and $0 < \delta < 1$ will be chosen at the very end of the computations; the specific mode k_{B_n} in each block will be chosen in the next stage of the computation.

Now we bound the ground state energy of the cutoff Hamiltonian (with the condition that the electronic co-ordinate of the ground-state wave function is localized) $\inf_{\|\Psi\|=1} \langle \Psi, H_K \Psi \rangle$, from below, using the energy of the *block Hamiltonian*:

$$\begin{aligned} & H_K^{\text{Block}}(\{k_{B_n}\}) \\ & = (1 - \epsilon)p^2 + (1 - \delta) \sum_{B_n} A_{B_n}^\dagger A_{B_n} - (P\alpha)^{\frac{1}{2}} \sum_{B_n} \left(A_{B_n} e^{ik_{B_n}x} + A_{B_n}^\dagger e^{-ik_{B_n}x} \right) - \alpha^2 V(\alpha x). \end{aligned} \quad (3.9)$$

Clearly,

$$\begin{aligned} H_K & = \left((1 - \epsilon)p^2 + \sum_{|k| < K} a_k^\dagger a_k - \left(\frac{\alpha}{L} \right)^{\frac{1}{2}} \sum_{B_n} \sum_{k \in B_n} \left(a_k e^{ik_{B_n}x} + a_k^\dagger e^{-ik_{B_n}x} \right) + \right. \\ & \quad \left. - \alpha^2 V(\alpha x) + \left(\frac{\alpha}{L} \right)^{\frac{1}{2}} \sum_{B_n} \sum_{k \in B_n} \left[a_k (e^{ik_{B_n}x} - e^{ikx}) + a_k^\dagger (e^{-ik_{B_n}x} - e^{-ikx}) \right] \right) \\ & \geq H_K^{\text{Block}}(\{k_{B_n}\}) - \frac{2\alpha K P^2 \pi^2}{\delta(\Delta E)}, \end{aligned} \quad (3.10)$$

in the sense of expectation values. To arrive at (3.10) we simply used the estimates from (3.7) and (3.8).

We summarize:

$$\inf_{\|\Psi\|=1} \langle \Psi, H_K \Psi \rangle \geq \inf_{\|\Psi\|=1} \sup_{\{k_{B_n}\}} \langle \Psi, H_K^{\text{Block}}(\{k_{B_n}\}) \Psi \rangle - \frac{2\alpha K P^2 \pi^2}{\delta(\Delta E)}.$$

3.4. Coherent States. We now work with the block Hamiltonian $H_K^{\text{Block}}(\{k_{B_n}\})$ from (3.9) and the block creation and annihilation operators constructed in the previous stage of the computation. For each block B_n we define a block coherent state indexed by some $z_{B_n} \in \mathbb{C}$:

$$|z_{B_n}\rangle = \pi^{-\frac{1}{2}} \left(e^{-\frac{|z_{B_n}|^2}{2} + z_{B_n} A_{B_n}^\dagger} \right) |0_{B_n}\rangle,$$

where $|0_{B_n}\rangle$ denotes the vacuum state in block B_n , i.e., $A_{B_n} |0_{B_n}\rangle = 0$. We write

$$|z\rangle = \prod_{B_n} |z_{B_n}\rangle,$$

a tensor product of the coherent states corresponding to each block B_n .

One can verify that for each block B_n , the coherent state $|z_{B_n}\rangle$ is the eigenstate of the corresponding block annihilation operator:

$$A_{B_n} |z_{B_n}\rangle = z_{B_n} |z_{B_n}\rangle.$$

The commutator relation $[A_{B_m}, A_{B_n}^\dagger] = \delta_{mn}$, together with the resolution of identity formula

$$I = \int |z\rangle \langle z| \prod_{B_m} dz_{B_m} d\bar{z}_{B_m},$$

yield the convenient representations:

$$\begin{aligned} A_{B_n} &= \int z_{B_n} |z\rangle \langle z| \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} \\ A_{B_n}^\dagger A_{B_n} &= \int (|z_{B_n}|^2 - 1) |z\rangle \langle z| \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} \end{aligned}$$

Denoting $\Psi_z(x) = \langle z | \Psi \rangle_{\text{Phonon}}$ (the inner product only in the phonon coordinates), we recast the energy of the block Hamiltonian $H_K^{\text{Block}}(\{k_{B_n}\})$ in the following form:

$$\langle \Psi, H_K^{\text{Block}}(\{k_{B_n}\}) \Psi \rangle = \int \langle \Psi_z, h_z \Psi_z \rangle_E \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} \quad (3.11)$$

where $\langle \cdot, \cdot \rangle_E$ is the inner product only over the electronic coordinate, and h_z is the Schrödinger operator:

$$h_z = (1 - \epsilon)p^2 + \sum_{B_n} \left[(1 - \delta) (|z_{B_n}|^2 - 1) - (P\alpha)^{\frac{1}{2}} (z_{B_n} e^{ik_{B_n}x} + \bar{z}_{B_n} e^{-ik_{B_n}x}) \right] - \alpha^2 V(\alpha x) \quad (3.12)$$

Since

$$\left(\langle \Psi_z, \Psi_z \rangle_E (1 - \delta) \bar{z}_{B_n} - (P\alpha)^{\frac{1}{2}} \langle \Psi_z, e^{ik_{B_n}x} \Psi_z \rangle_E \right) \left(z_{B_n} - \frac{(P\alpha)^{\frac{1}{2}}}{(1 - \delta) \langle \Psi_z, \Psi_z \rangle_E} \langle \Psi_z, e^{-ik_{B_n}x} \Psi_z \rangle_E \right) \geq 0,$$

completing the square yields

$$\begin{aligned} & (1 - \delta) \langle \Psi_z, \Psi_z \rangle_E |z_{B_n}|^2 - \bar{z}_{B_n} (P\alpha)^{\frac{1}{2}} \langle \Psi_z, e^{-ik_{B_n}x} \Psi_z \rangle_E - z_{B_n} (P\alpha)^{\frac{1}{2}} \langle \Psi_z, e^{ik_{B_n}x} \Psi_z \rangle_E \\ & \geq \frac{-(P\alpha) |\langle \Psi_z, e^{-ik_{B_n}x} \Psi_z \rangle_E|^2}{(1 - \delta) \langle \Psi_z, \Psi_z \rangle_E}. \end{aligned}$$

The advantage of constructing a Block Hamiltonian in the previous subsection is that the energy error we incur for disregarding the “-1” term in (3.12) is proportional to the number of blocks: $\frac{2K}{P}$, a finite value.

In the following calculation, in each block B_n we choose a mode \mathcal{K}_{B_n} such that

$$|\langle \Psi_z, e^{-i\mathcal{K}_{B_n}x} \Psi_z \rangle_E|^2 = \min_{k \in B_n} |\langle \Psi_z, e^{-ikx} \Psi_z \rangle_E|^2.$$

As seen in (3.15) below, we also make use of the continuum approximation $\sum_k \rightarrow L \int dk$ permitted by our model. We now proceed to extract the Pekar energy functional from (3.11):

$$\sup_{\{k_{B_n}\}} \langle \Psi, H_K^{\text{Block}}(\{k_{B_n}\}) \Psi \rangle$$

$$\geq \int \langle \Psi_z, \Psi_z \rangle_E \times \left((1-\epsilon) \frac{\langle \Psi_z, p^2 \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} - \frac{\alpha P}{(1-\delta)} \sum_{B_n} \frac{|\langle \Psi_z, e^{-iK B_n x} \Psi_z \rangle_E|^2}{|\langle \Psi_z, \Psi_z \rangle_E|^2} + \right. \\ \left. - \alpha^2 \frac{\langle \Psi_z, V(\alpha x) \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \quad (3.13)$$

$$= \int \langle \Psi_z, \Psi_z \rangle_E \times \left((1-\epsilon) \frac{\langle \Psi_z, p^2 \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} - \frac{\alpha}{(1-\delta)} \frac{1}{L} \sum_{B_n} \frac{(PL) |\langle \Psi_z, e^{-iK B_n x} \Psi_z \rangle_E|^2}{|\langle \Psi_z, \Psi_z \rangle_E|^2} + \right. \\ \left. - \alpha^2 \frac{\langle \Psi_z, V(\alpha x) \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \\ \geq \int \langle \Psi_z, \Psi_z \rangle_E \times \left((1-\epsilon) \frac{\langle \Psi_z, p^2 \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} - \frac{\alpha}{(1-\delta)} \frac{1}{L} \sum_k \frac{|\langle \Psi_z, e^{-ikx} \Psi_z \rangle_E|^2}{|\langle \Psi_z, \Psi_z \rangle_E|^2} + \right. \\ \left. - \alpha^2 \frac{\langle \Psi_z, V(\alpha x) \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \quad (3.14)$$

$$= \int \langle \Psi_z, \Psi_z \rangle_E \times \left((1-\epsilon) \frac{\langle \Psi_z, p^2 \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} - \frac{\alpha}{(1-\delta)} \int \left(\frac{|\langle \Psi_z, e^{-ikx} \Psi_z \rangle_E|^2}{|\langle \Psi_z, \Psi_z \rangle_E|^2} \right) dk + \right. \\ \left. - \alpha^2 \frac{\langle \Psi_z, V(\alpha x) \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \quad (3.15)$$

$$= \int \langle \Psi_z, \Psi_z \rangle_E \times \left((1-\epsilon) \frac{\langle \Psi_z, p^2 \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} - \frac{\alpha}{(1-\delta)} \int \left(\frac{|\Psi_z|^4}{|\langle \Psi_z, \Psi_z \rangle_E|^2} \right) dx + \right. \\ \left. - \alpha^2 \frac{\langle \Psi_z, V(\alpha x) \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \quad (3.16)$$

$$\geq \int \langle \Psi_z, \Psi_z \rangle_E \times (1-\epsilon) \left(\frac{\langle \Psi_z, p^2 \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} - \frac{\alpha}{(1-\delta)(1-\epsilon)} \int \left(\frac{|\Psi_z|^4}{|\langle \Psi_z, \Psi_z \rangle_E|^2} \right) dx + \right. \\ \left. - \frac{\alpha^2}{(1-\epsilon)^2(1-\delta)^2} \frac{\langle \Psi_z, V(\alpha x) \Psi_z \rangle_E}{\langle \Psi_z, \Psi_z \rangle_E} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \\ \geq \int \langle \Psi_z, \Psi_z \rangle_E \left(\frac{\alpha^2 e(V)}{(1-\epsilon)(1-\delta)^2} \right) \prod_{B_m} dz_{B_m} d\bar{z}_{B_m} - (1-\delta) \frac{2K}{P} \quad (3.17) \\ = \frac{\alpha^2 e(V)}{(1-\epsilon)(1-\delta)^2} - (1-\delta) \frac{2K}{P},$$

where $e(V)$ is the Pekar energy, defined in (2.5). Above (3.16) follows from the Plancherel's theorem, and (3.17) follows from the scaling properties of our Pekar functional.

3.5. Controlling the Error Terms. We have the following upper and lower bounds on the ground-state energy:

$$\alpha^2 e(V) \geq E_\alpha(V) \geq \frac{e(V)\alpha^2}{(1-\epsilon)(1-\delta)^2} - (1-\delta) \frac{2K}{P} - \frac{1}{2} - (\Delta E) - \frac{2\alpha K P^2 \pi^2}{\delta(\Delta E)} \quad (3.18) \\ = \alpha^2 e(V) - \underbrace{\left(\left(\frac{\alpha^2 \delta^2 - 2\alpha^2 \delta - \frac{8\alpha^3}{K} + \frac{16\alpha^3 \delta}{K} - \frac{8\alpha^3 \delta^2}{K} \right) e(V) - (1-\delta) \frac{2K}{P} - \frac{1}{2} - (\Delta E) - \frac{2\alpha K P^2 \pi^2}{\delta(\Delta E)} \right)}_{\text{error-term}},$$

since we noted, when using an ultraviolet cutoff above, that the parameters ϵ and K must satisfy the coupling relation: $\epsilon = \frac{8\alpha}{K}$. We now choose specific values (in orders of α) for the parameters K, δ, P and ΔE so that the error-term above is of an order less than α^2 , while satisfying the following constraints: $0 < \delta < 1$ and $P < K$ when $\alpha \gg 1$. In an attempt to make the error-term as small as possible, we have chosen

$$\delta = c_1 \alpha^{-\frac{1}{7}}, K = c_2 \alpha^{\frac{76}{49}}, P = c_3 \alpha^{\frac{5}{49}} \text{ and } \Delta E = c_4 \alpha^{\frac{64}{49}}.$$

From (3.18) we conclude

$$\alpha^2 e(V) \geq E_\alpha(V) \geq \alpha^2 e(V) - C \alpha^{\frac{71}{49}}.$$

This proves Theorem 1.

4. DIFFERENTIATING THE PEKAR ENERGY: PROOF OF LEMMA 5

Proof. Given any $\epsilon > 0$ and for any finite parameter $\delta > 0$, choose $u_\delta \in H^1(\mathbb{R})$ so that $\|u_\delta\|_2 = 1$, and

$$\int_{\mathbb{R}} (|u'_\delta|^2 - V(x)|u_\delta|^2 - |u_\delta|^4 + \delta W(x)|u_\delta|^2) dx - e(V + \delta W) < \epsilon \quad (4.1)$$

Since u_V is not necessarily the minimizer corresponding to the perturbed Pekar energy $e(V + \delta W)$,

$$\int_{\mathbb{R}} (|u'_\delta|^2 - V(x)|u_\delta|^2 - |u_\delta|^4 + \delta W(x)|u_\delta|^2) dx \leq \int_{\mathbb{R}} (|u'_V|^2 - V(x)|u_V|^2 - |u_V|^4 + \delta W(x)|u_V|^2) dx, \quad (4.2)$$

and

$$\delta \int_{\mathbb{R}} |u_V|^2 W(x) dx + e(V) \geq e(V + \delta W). \quad (4.3)$$

Since u_δ is not necessarily the minimizer corresponding to the Pekar energy $e(V)$,

$$\int_{\mathbb{R}} (|\nabla u_\delta|^2 + V(x)|u_\delta|^2 - |u_\delta|^4 + \delta W(x)|u_\delta|^2) dx \geq e(V) + \delta \int_{\mathbb{R}} |u_\delta|^2 W(x) dx, \quad (4.4)$$

and

$$\int_{\mathbb{R}} |u_V|^2 W(x) dx \geq \frac{e(V + \delta W) - e(V)}{\delta} \geq \int_{\mathbb{R}} |u_\delta|^2 W(x) dx \quad (4.5)$$

In parallel had we chosen $\delta < 0$ we would have arrived at the relation in (4.5) with the inequalities only reversed.

It suffices to show

$$\lim_{\delta \rightarrow 0} \int_{\mathbb{R}} |u_\delta|^2 W(x) dx = \int_{\mathbb{R}} |u_V|^2 W(x) dx, \quad (4.6)$$

where $W(x)$ is a bounded measure on the real line. We show this by arguing that u_δ converges uniformly to u_V on the real line.

In the limit $\delta \rightarrow 0$, the set of functions $\{u_\delta\}$ from (4.1) above is in fact a minimizing sequence of the Pekar functional \mathcal{E}_V (see (2.6)) with the Pekar energy $e(V)$. For δ small enough, since $e(V) < 0$,

$$\begin{aligned} 1 \geq 1 + e(V) &\geq \mathcal{E}_V(u_\delta) = \int_{\mathbb{R}} (|u'_\delta|^2 - |u_\delta|^4 - V(x)|u_\delta|^2) dx \\ &\geq \|u'_\delta\|_2^2 - \|u_\delta\|_\infty^2 - \|V\|_\infty \end{aligned} \quad (4.7)$$

$$\geq \frac{1}{2} \|u'_\delta\|_2^2 - \frac{1}{2} - \|V\|_\infty. \quad (4.8)$$

In (4.7) we use that $V \in C^1(\mathbb{R})$ and is a symmetric decreasing function. In (4.8) we use the one-dimensional Sobolev inequality, whence we have the uniform bound

$$\|u'_\delta\|_2^2 < 3 + 2\|V\|_\infty.$$

The sequence $\{u_\delta\}$ is thus uniformly bounded on $H^1(\mathbb{R})$, and $\{u_\delta\}$ - or a subsequence thereof- has a weak limit $u \in H^1(\mathbb{R})$.

Since V is a symmetric decreasing function, using rearrangement inequalities we see that given any $\epsilon > 0$, there is a compact set K_ϵ and a parameter $D_\epsilon > 0$ such that

$$\{x \in \mathbb{R} : |u_\delta|^2 \geq \epsilon \text{ for all } 0 < \delta < D_\epsilon\} \subseteq K_\epsilon. \quad (4.9)$$

Since V vanishes at infinity, we see that given any $\epsilon > 0$ there is a compact set K_ϵ such that

$$\{x \in \mathbb{R} : V(x) \geq \epsilon\} \subseteq K_\epsilon.$$

The compact set K_ϵ obviously has finite measure, so appealing to Theorem 8.6 in [LiLo] we conclude that the sequence $\{u_\delta\}$ converges to u *strongly* in $L^p(K_\epsilon)$ for all $p \leq \infty$, and that $\{u_\delta\}$ converges *pointwise uniformly* to u on K_ϵ . The latter convergence result follows from the fundamental theorem of calculus.

Thus,

$$-\int_{\mathbb{R}} |u_\delta|^2 V(x) dx - \int_{\mathbb{R}} |u_\delta|^4 dx \longrightarrow -\int_{\mathbb{R}} |u|^2 V(x) dx - \int_{\mathbb{R}} |u|^4 dx.$$

This establishes the weak lower semicontinuity of the Pekar functional \mathcal{E}_V , and the weak limit u is in fact the minimizer of \mathcal{E}_V . But we see from Proposition 3 above that \mathcal{E}_V admits a *unique* minimizer u_V , so $u \equiv u_V$.

Thus u_δ converges pointwise uniformly to u_V on K_ϵ , and from (4.9) we easily see that the convergence can be made uniform on the entire real line.

The relation in (4.6) now follows for any bounded measure $W(x)$ on the real line, and the perturbed Pekar energy $e(V + \delta W)$ is indeed differentiable at $\delta = 0$:

$$\lim_{\delta \rightarrow 0} \frac{e(V + \delta W) - e(V)}{\delta} = \int_{\mathbb{R}} |u_V|^2 W(x) dx.$$

□

5. PROOF OF THEOREM 4

In the proof, $\langle \cdot, \cdot \rangle$ should be read as the inner product on $\mathcal{F} \otimes L^2(\mathbb{R})$.

Proof. Recall the perturbed Hamiltonian $H_\alpha(V + \delta W)$ defined in (2.11):

$$H_\alpha(V + \delta W) = H_\alpha(V) + \alpha^2 \delta W(\alpha x)$$

and its ground state energy

$$E_\alpha(V + \delta W) = \alpha^2 e(V + \delta W)$$

discussed in (2.12)- (2.14).

Let Ψ_α be an approximate ground-state wave function (see Definition 2 above) of the Hamiltonian $H_\alpha(V)$ given in (2.1). From the variational principle,

$$E_\alpha(V + \delta W) - \langle \Psi_\alpha, H_\alpha(V) \Psi_\alpha \rangle \leq \alpha^2 \delta \langle \Psi_\alpha, W(\alpha x) \Psi_\alpha \rangle,$$

so that

$$\alpha^{-2} \{E_\alpha(V + \delta W) - \langle \Psi_\alpha, H_\alpha(V) \Psi_\alpha \rangle\} \leq \delta \langle \Psi_\alpha, W(\alpha x) \Psi_\alpha \rangle,$$

and

$$\liminf_{\alpha \rightarrow \infty} \alpha^{-2} \{E_\alpha(V + \delta W) - E_\alpha(V)\} \leq \delta \left(\liminf_{\alpha \rightarrow \infty} \langle \Psi_\alpha, W(\alpha x) \Psi_\alpha \rangle \right).$$

From Theorem 1 and (2.12) above,

$$e(V + \delta W) - e(V) \leq \delta \left(\liminf_{\alpha \rightarrow \infty} \left(\int_{\mathbb{R}} W(x) \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\circ}{\alpha} \right)\|_{\mathcal{F}}^2 \right] dx \right) \right).$$

For $\delta > 0$

$$\frac{e(V + \delta W) - e(V)}{\delta} \leq \liminf_{\alpha \rightarrow \infty} \int_{\mathbb{R}} W(x) \left(\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\circ}{\alpha} \right)\|_{\mathcal{F}}^2 \right) dx,$$

and

$$\lim_{\delta \rightarrow 0^+} \frac{e(V + \delta W) - e(V)}{\delta} \leq \liminf_{\alpha \rightarrow \infty} \left(\int_{\mathbb{R}} W(x) \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\circ}{\alpha} \right)\|_{\mathcal{F}}^2 \right] dx \right).$$

From Lemma 5,

$$\int_{\mathbb{R}} W(x) |u_V|^2 dx \leq \liminf_{\alpha \rightarrow \infty} \left(\int_{\mathbb{R}} W(x) \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\circ}{\alpha} \right)\|_{\mathcal{F}}^2 \right] dx \right).$$

For $\delta < 0$, we similarly arrive at the following relation:

$$\int_{\mathbb{R}} W(x) |u_V|^2 dx \geq \limsup_{\alpha \rightarrow \infty} \left(\int_{\mathbb{R}} W(x) \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\circ}{\alpha} \right)\|_{\mathcal{F}}^2 \right] dx \right).$$

We thus conclude:

$$\int_{\mathbb{R}} W(x) |u_V|^2 dx = \lim_{\alpha \rightarrow \infty} \left(\int_{\mathbb{R}} W(x) \left[\frac{1}{\alpha} \|\Psi_\alpha \left(\frac{\circ}{\alpha} \right)\|_{\mathcal{F}}^2 \right] dx \right),$$

which is our desired convergence relation for any approximate ground-state wave function with W a bounded measure on the real line. □

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